FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,916
APPLICANT Agrafiotis et al.	
FILING DATE March 12, 2001	GROUP 2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA1	4,773,099	09/1988	Bokser	382	14	
	AB1	4,811,217	03/1989	Tokizane et al.	364	300	
	AC1	4,859,736	08/1989	Rink	525	54.1	
	AD1	4,908,773	03/1990	Pantoliano et al.	364	496	
	AE1	4,935,875	06/1990	Shah et al.	364	497	
	AF1	4,939,666	07/1990	Hardman	364	496	
	AG1	5,010,175	04/1991	Rutter et al.	530	334	
	AH1	5,025,388	06/1991	Cramer, III et al.	364	496	
	AI1	5,155,801	10/1992	Lincoln	395	22	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AB	AJ1	EP 0 355 266 B1	02/1990	EPO	B01J	19/00	Yes No
	AK1	EP 0 355 628 B1	02/1990	EPO	G21F	9/00	No
	AL1	EP 0 770 876 A1	05/1997	EPO	G01N	33/68	Yes No
	AM1	EP 0 818 744 A2	01/1998	EPO	G06F	17/50	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	1	Borg, Ingwer and Groenen, Patrick, *Modern Multidimensional Scaling Theory and Applications*, Springer Series in Statistics, 1997, entire book submitted.
	AO	1	Agrafiotis, D.K. *et al.*, "Advances in diversity profiling and combinatorial series design," *Molecular Diversity*, Kluwer Academic Publishers, Vol. 4, 1999, pp. 1-22.
	AP	1	Agrafiotis, D.K. and Lobanov, V.S., "An Efficient Implementation of Distance-Based Diveristy Measures Based on *k-d* Trees," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 39, No. 1, January/February 1999, pp. 51-58.
	AQ	1	Agrafiotis, D.K. and Lobanov, V.S., "Bridging The Gap Between Diversity And QSAR," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 181-COMP.
	AR	1	Agrafiotis, D.K. and Jaeger, E.P., "Directed Diversity®: An Operating System For Combinatorial Chemistry," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 46-COMP.

EXAMINER	DATE CONSIDERED
Samuel Brooks	12/03/2003

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FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO.	APPLICATION NO.
1503.0200006	09/802,956
APPLICANT	
Agrafiotis et al.	
FILING DATE	GROUP
March 12, 2001	2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA2	5,167,009	11/1992	Skeirik	395	27	
	AB2	5,181,259	01/1993	Rorvig	382	36	
	AC2	5,240,680	08/1993	Zuckermann et al.	422	67	
	AD2	5,260,882	11/1993	Blanco et al.	364	499	
	AE2	5,265,030	11/1993	Skolnick et al.	364	496	
	AF2	5,270,170	12/1993	Schatz et al.	435	7.37	
	AG2	5,288,514	02/1994	Ellman	427	2	
	AH2	5,307,287	04/1994	Cramer, III et al.	364	496	
	AI2	5,323,471	06/1994	Hayashi	382	15	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AB	AJ2	WO 91/19735	12/1991	PCT	C07K	7/02	Yes No
	AK2	WO 92/00091	01/1992	PCT	A61K	37/02	Yes No
	AL2	WO 93/20242	10/1993	PCT	C12Q	1/70	Yes No
	AM2	WO 94/28504	12/1994	PCT	G06F	15/60	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	2	Agrafiotis, D.K., "Diversity of Chemical Libraries," *Encyclopedia of Computational Chemistry*, John Wiley & Sons Ltd, Vol. 1:A-D, 1998, pp. 742-761.
	AO	2	Agrafiotis, D.K., "On the Use of Information Theory for Assessing Molecular Diversity," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 37, No. 3, May/June 1997, pp. 576-580.
	AP	2	Agrafiotis, D.K. *et al.*, "Parallel QSAR," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 50-COMP.
	AQ	2	Agrafiotis, D.K. *et al.*, "PRODEN: A New Program for Calculating Integrated Projected Populations," *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 11, No. 9, October 1990, pp. 1101-1110.
	AR	2	Agrafiotis, D.K. and Jaeger, E.P., "Stochastic Algorithms for Exploring Molecular Diversity," *Abstracts of Papers Part 1: 213th ACS National Meeting*, April 13-17, 1997, p. 16-CINF.

EXAMINER	DATE CONSIDERED
Samuel Brooks	12/03/03

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1503.0200006	09/802,956
APPLICANT: Agrafiotis et al.	
FILING DATE: March 12, 2001	GROUP: 2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AK	AA3	5,331,573	07/1994	Balaji et al.	364	500	
	AB3	5,434,796	07/1995	Weininger	364	496	
	AC3	5,436,850	07/1995	Eisenberg et al.	364	496	
	AD3	5,442,122	08/1995	Noda et al.	564	426	
	AE3	5,463,564	10/1995	Agrafiotis et al.	364	496	
	AF3	5,499,193	03/1996	Sugawara et al.	364	500	
	AG3	5,519,635	05/1996	Miyake et al.	364	497	
	AH3	5,524,065	06/1996	Yagasaki	382	226	
	AI3	5,526,281	06/1996	Chapman et al.	364	496	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AK	AJ3	WO 95/01606	01/1995	PCT	G06F	15/42	Yes No
	AK3	WO 97/09342	03/1997	PCT	C07H	21/02	Yes No
	AL3	WO 97/20952	06/1997	PCT	C12Q	1/68	Yes No
	AM3	WO 97/27559	07/1997	PCT	G06F	19/00	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AK	AN	3	Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies - Applications and Impacts *Information Processing '94*, North-Holland, Vol. II, 1994, pp. 714-719.
	AO	3	Biswas, G. *et al.*, "Evaluation of Projection Algorithms," *IEEE Transactions On Pattern Analysis And Machine Intelligence*, IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708.
	AP	3	Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517-4533.
	AQ	3	Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," *IEEE Transactions on Systems, Man, and Cybernetics*, IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, March 1973, pp. 197-200.
	AR	3	Cramer, R.D. *et al.*, "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 38, No. 6, November/December 1998, pp. 1010-1023.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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APPLICANT Agrafiotis et al.	
FILING DATE March 12, 2001	GROUP 2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA4	5,545,568	08/1996	Ellman	436	518	
	AB4	5,549,974	08/1996	Holmes	428	403	
	AC4	5,553,225	09/1996	Perry	395	157	
	AD4	5,565,325	10/1996	Blake	435	7.1	
	AE4	5,574,656	11/1996	Agrafiotis et al.	364	500	
	AF4	5,585,277	12/1996	Bowie et al.	436	518	
	AG4	5,602,755	02/1997	Ashe et al.	364	498	
	AH4	5,602,938	02/1997	Akiyama et al.	382	155	
	AI4	5,612,895	03/1997	Balaji et al.	364	496	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AB	AJ4	WO 98/20437	05/1998	PCT	G06F	17/50	Yes No
	AK4	WO 98/20459	05/1998	PCT	G06T	11/20	Yes No
	AL4						Yes No
	AM4						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	4	DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," *Advances in Neural Information Processing Systems*, Vol. 5, 1993, pp. 580-587.
	AO	4	Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," *Machine Learning*, Kluwer Academic Publishers, Vol. 6, 1991, pp. 161-182.
	AP	4	Friedman, J.H., "Exploratory Projection Pursuit," *Journal of the American Statistical Association*, Am rican Statistical Association, Vol. 82, No. 397, March 1987, pp. 249-266.
	AQ	4	Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," *IEEE Transactions on Computers*, IEEE Computer Society, Vol. C-23, No. 9, September 1974, pp. 881-889.
	AR	4	Garrido, L. *et al.*, "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," *International Journal of Neural Systems*, World Scientific Publishing Co. Pte. Ltd., Vol. 6, No. 3, September 1995, pp. 273-282.

EXAMINER	DATE CONSIDERED
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AN	AA5	5,634,017	05/1997	Mohanty et al.	395	326	
	AB5	5,635,598	06/1997	Lebl et al.	530	334	
	AC5	5,670,326	09/1997	Beutel	435	7.1	
	AD5	5,679,582	10/1997	Bowie et al.	436	518	
	AE5	5,684,711	11/1997	Agrafiotis et al.	364	500	
	AF5	5,703,792	12/1997	Chapman	364	496	
	AG5	5,712,171	01/1998	Zambias et al.	436	518	
	AH5	5,712,564	01/1998	Hayosh	324	210	
	AI5	5,736,412	04/1998	Zambias et al.	436	518	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ5						Yes No
	AK5						Yes No
	AL5						Yes No
	AM5						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AN	AN	5	Ghose, A.K. *et al.*, "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," *J. Phys. Chem. A*, American Chemical Society, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772.
	AO	5	Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-Property Modeling," *Reviews in Computational Chemistry: Advances*, VCH Publishers, Inc., 1991, pp. 367-422.
	AP	5	Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," *Science*, American Association for the Advancement of Science, Vol. 269, September 29, 1995, pp. 1860-1863.
	AQ	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 6, September 1933, pp. 417-441.
	AR	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 7, October 1933, pp. 498-520.

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Agrafiotis et al.	
FILING DATE	GROUP
March 12, 2001	2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
MB	AA6	5,740,326	04/1998	Boulet et al.	395	27	
	AB6	5,789,160	08/1998	Eaton et al.	435	6	
	AC6	5,807,754	09/1998	Zambias et al.	436	518	
	AD6	5,811,241	09/1998	Goodfellow et al.	435	7.1	
	AE6	5,832,494	11/1998	Egger et al.	707	102	
	AF6	5,858,660	01/1999	Eaton et al.	435	6	
	AG6	5,861,532	01/1999	Brown et al.	564	142	
	AH6	5,866,334	02/1999	Beutel	435	6	
	AI6	5,901,069	05/1999	Agrafiotis et al.	364	528.03	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ6						No
	AK6						Yes No
	AL6						Yes No
	AM6						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MB	AN	6	Lee, R.C.T. *et al.*, "A Triangulation Method for the Sequential Mapping of Points from *N*-Space to Two-Space," *IEEE Transactions on Computers*, The Institute of Electrical and Electronics Engineers, March 1977, pp. 288-292.
	AO	6	Lipinski, C.A. *et al.*, "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," *Advanced Drug Delivery Reviews*, Elsevier Science B.V., Vol. 23, 1997, pp. 3-25.
	AP	6	Lobanov, V.S. and Agrafiotis, D.K., "Intelligent Database Mining Techniques," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 19-COMP.
	AQ	6	Lobanov, V.S. *et al.*, "Rational Selections from Virtual Libraries," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 181-COMP.
	AR	6	Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," *IEEE transactions on Neural Networks*, IEEE Neural Networks, Vol. 6, No. 2, March 1995, pp. 296-317.

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Samuel Broda	12/03/03

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
NB	AA7	5,908,960	06/1999	Newlander	564	177	
	AB7	5,993,819	11/1999	Haynes et al.	424	188.1	
	AC7	6,014,661	01/2000	Ahlberg et al.	707	3	
	AD7	6,037,135	03/2000	Kubo et al.	435	7.24	
	AE7	6,049,797	04/2000	Guha et al.	707	6	
	AF7	6,185,506 B1	02/2001	Cramer et al.	702	19	
	AG7						
	AH7						
	AI7						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ7						Yes / No
	AK7						No
	AL7						Yes / No
	AM7						Yes / No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	7	Oja, E., "Principal Components, Minor Components, and Linear Neural Networks," *Neural Networks*, Pergamon Press Ltd., Vol. 5, 1992, pp. 927-935.
	AO	7	Patterson, D.E. *et al.*, "Neighborhood Behavior: A Useful Concept for Validation of 'Molecular Diversity' Descriptors," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 39, No. 16, 1996, pp. 3049-3059.
	AP	7	Pykett, C.E., "Improving the Efficiency of Sammon's Nonlinear Mapping by Using Clustering Archetypes," *Electronics Letters*, The Institute of Electrical Engineers, Vol. 14, No. 25, December 7, 1978, pp. 799-800.
	AQ	7	Rubner, J. and Tavan, P., "A Self-Organizing Network for Principal-Component Analysis," *Europhysics Letters*, European Physical Society, Vol. 10, No. 7, December 1, 1989, pp. 693-698.
	AR	7	Sadowski, J. *et al.*, "Assessing Similarity and Diversity of Combinatorial Libraries by Spatial Autocorrelation Functions and Neural Networks," *Angewandte Cheme*, VCH, Vol. 34, No. 23/24, January 5, 1996, pp. 2674-2677.

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Samuel Broda	12/03/03

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA8						
	AB8						
	AC8						
	AD8						
	AE8						
	AF8						
	AG8						
	AH8						
	AI8						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ8						No
	AK8						No
	AL8						No
	AM8						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	8	Thompson, L.A. and Ellman, J.A., "Synthesis and Applications of Small Molecule Libraries," *Chemical Reviews*, American Chemical Society, Vol. 96, No. 1, January/February 1996, pp. 555-600.
	AO	8	Barnard, John M. and Downs, Geoff M., "Computer representation and manipulation of combinatorial libraries," *Perspectives in Drug Discovery and Design*, Kluwer Academic Publishers, 1997, pp. 13-30.
	AP	8	Brint, Andrew T. and Willett, Peter, "Upperbound procedures for the identification of similar three-dim nsional chemical structures," *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 2, No. 4, January 1989, pp. 311-320.
	AQ	8	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 40, No. 15, 1997, pp. 2304-2313.
	AR	8	Gillet, Valerie J. *et al.*, "The Effectiveness of Reactant Pools for Generating Structurally-Diverse Combinatorial Libraries," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 37, No. 4, 1997, pp. 731-740.

EXAMINER: Samuel Brooks — DATE CONSIDERED: 12/03/03

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA9						
	AB9						
	AC9						
	AD9						
	AE9						
	AF9						
	AG9						
	AH9						
	AI9						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ9						Yes No
	AK9						Yes No
	AL9						Yes No
	AM9						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	9	Gillet, Valerie J. *et al.*, "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 39, No. 1, 1999, pp. 169-177.
	AO	9	Kearsley, Simon K. *et al.*, "Chemical Similarity Using Physiochemical Property Descriptors," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 118-127.
	AP	9	Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 37, No. 1, 1997, pp. 62-70.
	AQ	9	Lewis, Richard A. *et al.*, "Similarity Measures for Rational Set Selection and Analysis of Combinatorial Libraries: The Diverse Property-Derived (DPD) Approach," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 37, No. 3, 1997, pp. 599-614.
	AR	9	Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug Discovery," *Journal of Combinatorial Chemistry*, American Chemical Society, Vol. 1, No. 1, 1999, pp. 32-45.

EXAMINER	DATE CONSIDERED
Samuel Brody	12/03/03

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APPLICANT: Agrafiotis et al.	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA10						
	AB10						
	AC10						
	AD10						
	AE10						
	AF10						
	AG10						
	AH10						
	AI10						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ10						Yes No
	AK10						Yes No
	AL10						Yes No
	AM10						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	10	Sheridan, Robert P. *et al.*, "Chemical Similarity Using Geometric Atom Pair Descriptors," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 128-136.
↓	AO	10	Willett, Peter *et al.*, "Chemical Similarity Searching," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 38, No. 6, 1998, pp. 983-996.
↓	AP	10	Agrafiotis, Dimitris K. and Lobanov, Victor S., "Ultrafast Algorithm for Designing Focused Combinational Arrays," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 2000, Vol. 40, No. 4, pp. 1030-1038.
AB	AQ	10	Ajay *et al.*, "Can We Learn To Distinguish between 'Drug-Like' and 'Nondrug-like' Molecules?" *J. Med. Chem.*, 1998, American Chemical Society, Vol. 41, No. 18, pp. 3314-3324.
AB	AR	10	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *J. Med. Chem.*, American Chemical Society, 1997, Vol. 40, No. 15, pp. 2304-2313.

EXAMINER: Samuel Kassa — DATE CONSIDERED: 12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA11						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ11						N/A
	AK11						Yes (See AP50)
	AL11						Yes (See AR50)
	AM11						Yes (See AN51)

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	11	Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors Relevant to Ligand-Receptor Binding," *J. Chem. Info. Comput. Sci.*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 1-9.
	AO	11	Brown, Robert D. and Martin, Yvonne C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," *J. Chem. Inf. Sci.*, American Chemical Society, 1996, Vol. 36, No. 3, pp. 572-584.
	AP	11	Cummins, David J. *et al.*, "Molecular Diversity in Chemical Databases: Comparison of Medicinal Chemistry Knowledge Bases and Databases of Commercially Available Compounds," *J. Chem. Info. Comput. Sci.*, American Chemical Society, 1996, Vol. 36, No. 4, pp. 750-763.
	AQ	11	*Daylight Theory: Fingerprints* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.finger.html>, 9 pages.
	AR	11	*Daylight Theory: SMARTS* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html>, 10 pages.

EXAMINER	DATE CONSIDERED
Samuel Broda	

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FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO.	APPLICATION NO.
1503.0200006	09/802,956
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA12						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ12						
	AK12						
	AL12						
	AM12						

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	12	Downs, Geoff M. and Barnard, John M., "Techniques for Generating Descriptive Fingerprints in Combinatorial Libraries," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 59-61.
	AO	12	Gillet, Valerie J., "Background Theory of Molecular Diversity," *Molecular Diversity in Drug Design*, Kluwer Academic Publishers, 1999, pp. 43-65.
	AP	12	Good, Andrew C. and Lewis, Richard A., "New Methodology for Profiling Combinatorial Libraries and Screening Sets: Cleaning Up the Design Process with HARPick," *J. Med. Chem.*, American Chemical Society, 1997, Vol. 40, No. 24, pp. 3926-3936.
	AQ	12	Gorse, Dominique and Lahana, Roger, "Functional diversity of compound libraries," *Current opinion in chemical biology*, Elsevier Science Ltd., June 2000, Vol. 4, No. 3, pp. 287-294.
	AR	12	Jamois, Eric A. *et al.*, "Evaluation of Reagent-Based and Product-Based Strategies in the Design of Combinatorial Library Subsets," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 2000, Vol. 40, No.1, pp. 63-70.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA13						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ13						
	AK13						
	AL13						
	AM13						

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	13	Leach, Andrew R. *et al.*, "Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Design," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 1999, Vol. 39, No. 6, pp. 1161-1172.
AB	AO	13	Leach, Andrew R. and Hann, Michael M., "The *in silico* world of virtual libraries," *Drug discovery today*, Elsevier Science Ltd., August 2000, Vol. 5, No. 8, pp. 326-336.
	AP	13	~~Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *J. Chem. Inf. Comput. Sci.*, American~~ Chemical Society, 1997, Vol. 37, No. 1, pp. 62-70.
AB	AQ	13	Lobanov, Victor S. and Agrafiotis, Dimitris K., "Stochastic Similarity Selections from Large Combinatorial Libraries," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, March/April 2000, Vol. 40, No. 2, pp. 460-470.
↓	AR	13	Matter, Hans and Pötter, Thorsten, "Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 1999, Vol. 39, No. 6, pp. 1211-1225.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA14						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ14						No
	AK14						No
	AL14						No
	AM14						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	14	Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors," *J. Med. Chem.*, American Chemical Society, 1997, Vol. 40, No. 8, pp. 1219-1229.
	AO	14	Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," *J. Med. Chem.*, American Chemical Society, 1998, Vol. 41, No. 18, pp. 3325-3329.
	AP	14	Schnur, Dora, "Design and Diversity Analysis of Large Combinatorial Libraries Using Cell-Based Methods," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 1999, Vol. 39, No. 1, pp. 36-45.
	AQ	14	Schuffenhauer, Ansgar *et al.*, "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, 2000, Vol. 40, No. 2, pp. 295-307.
	AR	14	Turner, David B. *et al.*, "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," *J. Chem. Inf. Sci.*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 18-22.

EXAMINER Samuel Brooks — DATE CONSIDERED 12/03/03

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA15						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ15						No
	AK15						No
	AL15						No
	AM15						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	15	Wang, Jing and Ramnarayan, Kal, "Toward Designing Drug-Like Libraries: A Novel Computational Approach for Prediction of Drug Feasibility of Compounds," *J. Comb. Chem.*, American Chemical Society, November/December 1999, Vol. 1, No. 6, pp. 524-533.
	AO	15	Gasteiger, J. *et al*, "Assessment of the Diversity of Combinatorial Libraries by an Encoding of Molecular Surface Properties," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 70-CINF.
	AP	15	Hassan, Moises *et al.*, "Optimization and visualization of molecular diversity of combinatorial libraries," *Molecular Diversity*, ESCOM Science Publishers B.V., 1996, Vol. 2, pp. 64-74.
	AQ	15	Bellman, R.E., *Adaptive Control Processes: A Guided Tour*, Princeton Univ. Press, Princeton, NJ (1961).
	AR	15	Bezdek, J.C., *Pattern Recognition with Fuzzy Objective Function Algorithms*, Plenum Press, New York, NY (1981).

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA16						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ16						No
	AK16						No
	AL16						No
	AM16						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MB	AN	16	Johnson, M.A., and Maggiora, G.M., *Concepts and Applications of Molecular Similarity*, John Wiley and Sons, New York, NY (1990).
	AO	16	Kohonen, T., *Self-Organizing Maps*, Springer-Verlag, Heidelberg, Germany (1995).
	AP	16	Oja, E., *Subspace Methods of Pattern Recognition*, Research Studies Press, Letchworth, England (1983).
	AQ	16	Agrafiotis, D.K., "A New Method For Analyzing Protein Sequence Relationships Based On Sammon Maps," *Protein Science*, Cambridge University Press, Vol. 6, No. 2, February 1997, pp. 287-293.
	AR	16	Copy of International Search Report issued October 18, 1999, for Appl. No. PCT/US99/09963, 7 pages.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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	AA17						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ17						No
	AK17						No
	AL17						No
	AM17						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	17	Amzel, L.M., "Structure-based drug design," *Current Opinion in Biotechnology*, Vol. 9, No. 4, August 1998, pp. 366-369.
	AO	17	Blaney, J.M. and Martin, E.J., "Computational approaches for combinatorial library design and molecular diversity analysis," *Current Opinion in Chemical Biology*, Current Biology Ltd., Vol. 1, No. 1, June 1997, pp. 54-59.
	AP	17	Brown, R.D. and Clark, D.E., "Genetic diversity: applications of evolutionary algorithms to combinatorial library design," *Expert Opinion on Therapeutic Patents*, Vol. 8, No. 11, November 1998, pp. 1447-1459.
	AQ	17	Caflisch, A. and Karplus, M., "Computational combinatorial chemistry for de novo ligand design: Review and assessment," *Perspectives in Drug Discovery and Design*, ESCOM Science Publishers B.V., Vol. 3, 1995, pp. 51-84.
	AR	17	Danheiser, S.L., "Current Trends in Synthetic Peptide and Chemical Diversity Library Design," *Genetic Engineering News*, May 1, 1994, pp. 10 and 31.

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Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA18						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ18						Yes No
	AK18						Yes No
	AL18						Yes No
	AM18						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	18	Eichler, U. *et al.*, "Addressing the problem of molecular diversity," *Drugs of the Future*, Prous Science, Vol. 24, No. 2, 1999, pp. 177-190.
	AO	18	Felder, E.R. and Poppinger, D., "Combinatorial Compound Libraries for Enhanced Drug Discovery Approaches," *Advances in Drug Research*, Academic Press, Vol. 30, 1997, pp. 112-199.
	AP	18	Geysen, H.M. and Mason, T.J., "Screening Chemically Synthesized Peptide Libraries for Biologically-Relevant Molecules," *Biorganic & Medicinal Chemistry Letters*, Pergamon Press Ltd., Vol. 3, No. 3, 1993, pp. 397-404.
	AQ	18	Gobbi, A. *et al.*, "New Leads By Selective Screening of Compounds From Large Databases," *Abstracts of Papers Part 1: 213th ACS National Meeting*, April 13-17, 1997, p. 67-CINF.
	AR	18	Houghten, R.A. *et al.*, "The Use of Synthetic Peptide Combinatorial Libraries for the Identification of Bioactive Peptides," *Peptide Research*, Vol. 5, No. 6, 1992, pp. 351-358.

EXAMINER	DATE CONSIDERED
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA19						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ19						Yes No
	AK19						Yes No
	AL19						Yes No
	AM19						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	19	Klopman, G., "Artificial Intelligence Approach to Structure-Activity Studies. Computer Automated Structure Evaluation of Biological Activity of Organic Molecules," *J. Am. Chem. Soc.*, American Chemical Society, Vol. 106, No. 24, November 28, 1984, pp. 7315-7321.
	AO	19	Lajiness, M.S. *et al.*, "Implementing Drug Screening Programs Using Molecular Similarity Methods," *QSAR: Quantitative Structure-Activity Relationships in Drug Design*, Alan R. Liss, Inc., 1989, pp. 173-176.
	AP	19	Loew, G.H. *et al.*, "Strategies for Indirect Computer-Aided Drug Design," *Pharmaceutical Research*, Plenum Publishing Corporation, Vol. 10, No. 4, 1993, pp. 475-486.
	AQ	19	Lynch, M.F. *et al.*, "Generic Structure Storage and Retrieval," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 25, No. 3, August 1985, pp. 264-270.
	AR	19	Myers, P.L. *et al.*, "Rapid, Reliable Drug Discovery," *Today's Chemist At Work*, American Chemical Society, Vol. 6, No. 7, July/August 1997, pp. 46-48, 51 & 53.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA20						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ20						Yes No
	AK20						Yes No
	AL20						Yes No
	AM20						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	20	Pabo, C.O. and Suchanek, E.G., "Computer-Aided Model-Building Strategies for Protein Design," *Biochemistry*, American Chemical Society, Vol. 25, No. 20, 1986, pp. 5987-5991.
	AO	20	Saudek, V. *et al.*, "Solution Conformation of Endothelin-1 by H NMR, CD, and Molecular Modeling," *International Journal of Peptide Protein Res.*, Munksgaard International Publishers Ltd., Vol. 37, No. 3, 1991, pp. 174-179.
	AP	20	Singh, J. *et al.*, "Application of Genetic Algorithms to Combinatorial Synthesis: A Computational Approach to Lead Identification and Lead Optimization," *J. Am. Chem. Soc.*, American Chemical Society, Vol. 118, No. 5, February 7, 1996, pp. 1669-1676.
	AQ	20	Van Drie, J.H. and Lajiness, M.S., "Approaches to virtual library design," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 6, June 1998, pp. 274-283.
	AR	20	Walters, W.P. *et al.*, "Virtual screening - an overview," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 4, April 1998, pp. 160-178.

EXAMINER	DATE CONSIDERED
Samuel Weeks	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA21						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ21						Yes No
	AK21						Yes No
	AL21						Yes No
	AM21						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	21	Weber, L., "Evolutionary combinatorial chemistry: application of genetic algorithms," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 8, August 1998, pp. 379-385.
	AO	21	Weber, L. *et al.*, "Optimization of the Biological Activity of Combinatorial Compound Libraries by a Genetic Algorithm," *Angewandte Chemie International Edition in English*, VCH, Vol. 34, No. 20, November 3, 1995, pp. 2280-2282.
	AP	21	Graybill, T.L. *et al.*, "Enhancing the Drug Discovery Process by Integration of High-Throughput Chemistry and Structure-Based Drug Design," from Molecular Diversity and Combinatorial Chemistry: Libraries and Drug Discovery, Chaiken and Janda (eds.), American Chemical Society, 1996, pp. 16-27.
	AQ	21	Saund, E., "Dimensionality-Reduction Using Connectionist Networks," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, IEEE, Vol. 11, No. 3, March 1989, pp. 304-314.
	AR	21	"3DP gains drug research patent", Chemistry in Britain, The Royal Society of Chemistry, Vol. 32, No. 1, January 1996, p. 22.

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ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,9[illegible]
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA22						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ22						Yes No
	AK22						Yes No
	AL22						Yes No
	AM22						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	22	"Accelerate the Discovery Cycle with Chem-X!", Source and date of publication unclear, 2 pages.
	AO	22	Agrafiotis, D. K., "Stochastic Algorithms for Maximizing Molecular Diversity", *Journal of Chemical Information and Computer Sciences,* American Chemical Society, Vol. 37, No. 5, 1997, pp. 841-851.
	AP	22	Alsberg, B.K. *et al.*, "Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, *K*-nearest neighbour, neural and decision-tree methods", *Analytica Chimica Acta*, Elsevier Science B.V., Vol. 348, No. 1-3, August 20, 1997, pp. 389-407.
	AQ	22	Andrea, T.A. and Kalayeh, H., "Applications of Neural Networks in Quantitative Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 34, No. 9, 1991, pp. 2824-2836.
	AR	22	Aoyama, T. *et al.*, "Neural Networks Applied to Quantitative Structure-Activity Relationship Analysis", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 9, 1990, pp. 2583-2590.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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	AA23						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ23						Yes No
	AK23						Yes No
	AL23						Yes No
	AM23						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	23	Aoyama, T. and Ichikawa, H., "Obtaining the Correlation Indices between Drug Activity and Structural Parameters Using a Neural Network", *Chemical & Pharmaceutical Bulletin*, Pharmaceutical Society of Japan, Vol. 39, No. 2, February 1991, pp. 372-378.
	AO	23	"ArQule Inc", from *http://www.bioportfolio.com/arqule/products.htm*, 5 pages, (March 18, 1998).
	AP	23	Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry", *Chemical & Engineering News*, American Chemical Society, February 7, 1994, pp. 20-26.
	AQ	23	Bentley, J. L., "Multidimensional Binary Search Trees Used for Associative Searching", *Communications of the ACM*, Association for Computing Machinery, Inc., Vol. 18, No. 9, September 1975, pp. 509-517.
	AR	23	Bottou, L. and Vladimir Vapnik, "Local Learning Algorithms", *Neural Computation*, Massachusetts Institute of Technology, Vol. 4, No. 6, pp. 888-900, (November 1992).

EXAMINER	DATE CONSIDERED
Samuel Kyoka	12/03/03

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,956
APPLICANT Agrafiotis et al.	
FILING DATE March 12, 2001	GROUP 2123

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA24						
	AB24						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ24						Yes No
	AK24						Yes No
	AL24						Yes No
	AM24						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	24	Boulu, L.G. and Crippen, G.M., "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 10, No. 5, July/August 1989, pp. 673-682.
	AO	24	Boulu, L.G. *et al.*, "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 2, 1990, pp. 771-775.
	AP	24	Brown, R. D. and Martin, Y.C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection", *Journal of Chemical Information and Computer Sciences*, Vol. 36, No. 3, 1996, pp. 572-584.
AB	AQ	24	Cacoullos, T., "Estimation of a Multivariate Density", *Annals of The Institute of Statistical Mathematics*, The Institute of Statistical Mathematics, Vol. 18, No. 2, 1966, pp. 179-189.
	AR	24	Clark, R.D., "OptiSim: An Extended Dissimilarity Selection Method for Finding Diverse Representative Subsets", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 6, 1997, pp. 1181-1188.

EXAMINER	DATE CONSIDERED
Samuel Kosh	12/03/05

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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APPLICANT: Agrafiotis et al.	
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA25						
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	AI25						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ25						Yes No
	AK25						Yes No
	AL25						Yes No
	AM25						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	25	Clark, D. E., and Westhead, D.R., "Evolutionary algorithms in computer-aided molecular design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 10, No. 4, August 1996, pp. 337-358.
	AO	25	Cramer, III, R. D. *et al.*, "Comparative Molecular Field Analyisis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins", *Journal of The American Chemical Society*, American Chemical Society, Vol. 110, No. 18, August 31, 1988, pp. 5959-5967.
	AP	25	Cramer, III, R. D. *et al.*, "Substructural Analysis. A Novel Approach to the Problem of Drug Design", *Journal of Medicinal Chemistry*, Vol. 17, No. 5, May 1974, pp. 533-535.
	AQ	25	Crippen, G. M., "Voronoi Binding Site Models", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 8, No. 7, October/November 1987, pp. 943-955.
	AR	25	Friedman, J. H. *et al.*, "An Algorithm for Finding Best Matches in Logarithmic Expected Time", *ACM Transactions on Mathematical Software*, Association for Computing Machinery, Vol. 3, No. 3, September 1977, pp. 209-226.

EXAMINER: Samuel Gregory — DATE CONSIDERED: 12/03/03

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA26						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ26						Yes No
	AK26						Yes No
	AL26						Yes No
	AM26						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	26	Friedman, J.H., "Fitting Functions To Noisy Data In High Dimensions", Department of Statistics- Stanford University Technical Report No. 101, (August, 1988).
	AO	26	Gallop, M. A. *et al.*, "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 37, No. 9, April 29, 1994, pp. 1233-1251.
	AP	26	Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Qantitative Structure-Activity Relationships: A Demonstration Using *Escherichia coli* Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 28, No. 3, 1985, pp. 333-346.
	AQ	26	Good, A. C. *et al.*, "Structure-Activity Relationships from Molecular Similarity Matrices", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438.
	AR	26	Gordon, E. M. *et al.*, "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA27						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ27						Yes No
	AK27						Yes No
	AL27						Yes No
	AM27						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	27	Hartigan, J. A., "Representation of Similarity Matrices By Trees", *Journal of the American Statistical Association*, Vol. 62, No. 320, December, 1967, pp. 1140-1158.
	AO	27	Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based upon Molecular Shape Analysis", *Journal of the American Chemical Society*, American Chemical Society, Vol. 102, No. 24, November 19, 1980, pp. 7196-7206.
	AP	27	Jackson, R. C., "Update on computer-aided drug design", *Current Opinion in BIOTECHNOLOGY*, Current Biology Ltd., Vol. 6, No. 6, December 1995, pp. 646-651.
	AQ	27	Kim, K. H., "Comparative molecular field analysis (CoMFA)", *Molecular Similarity in Drug Design*, ed. P. M. Dean, Blackie Academic & Professional, 1995, Ch. 12, pp. 291-331.
	AR	27	Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", *Biological Cybernetics*, Springer-Verlag, Vol. 43, No. 1, 1982, pp. 59-69.

EXAMINER: Samuel Broda — DATE CONSIDERED: 12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA28						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ28						Yes No
	AK28						Yes No
	AL28						Yes No
	AM28						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	28	Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", *Proceedings of the 25h Hawaii International Conference on System Sciences*, IEEE, 1992, pp. 706-716.
	AO	28	Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", *Journal of the American Chemical Society*, American Chemical Society, Vol. 95, No. 3, February 7, 1973, pp. 686-693.
	AP	28	Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", *Psychometrika*, Vol. 29, No. 2, June, 1964, pp. 115-129.
	AQ	28	Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", *Current Opinion in Structural Biology*, Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406.
	AR	28	Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 34, No. 6, November/December 1994, pp. 1279-1287.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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	AA29						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ29						Yes No
	AK29						Yes No
	AL29						Yes No
	AM29						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MB	AN	29	Martin, E. J. *et al.*, "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", *Reviews in Computational Chemistry*, VCH Publishers, Inc., Vol. 10, 1997, pp. 75-99.
	AO	29	Martin, E. J. *et al.*, "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 38, No. 9, April 28, 1995, pp. 1431-1436.
	AP	29	McMartin, C. and Bohacek, R.S., "QXP: Powerful, rapid computer algorithms for structure-based drug design", *Journal of Computer-Aided Molecular Design*, Kluwer Academic Publishers, Vol. 11, No. 4, July 1997, pp. 333-344.
	AQ	29	Mezey, P. G. and Walker, P.D., "Fuzzy molecular fragments in drug research", *Drug Discovery today*, Vol. 2, No. 4, April 1997, pp. 132-137.
	AR	29	Müller, K., "On the paradigm shift from rational to random design", *Journal of Molecular Structure (Theochem)*, Elsevier Science B.V., Vol. 398-399, Special Issue, 1997, pp. 467-471.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA30						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ30						Yes No
	AK30						Yes No
	AL30						Yes No
	AM30						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	30	Myers, P., "The Design Of A Universal, Informer™ Library", COMBICHEM, INC., 10 Pages, Date unknown.
	AO	30	Oinuma, H. *et al.*, "Neural Networks Applied to Structure-Activity Relationships", *Journal of Medicinal Chemistry*, Vol. 33, No. 3, pp. 905-908, (1990).
	AP	30	Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", *Advances in Neural Information Processing Systems 3*, Morgan Kaufmann, 1991, 7 pages, unknown.
	AQ	30	Parrill, A. L., "Evolutionary and genetic methods in drug design", *Drug Discovery today*, Elsevier Science Ltd., Vol. 1, No. 12, December 1996, pp. 514-521.
	AR	30	Polanski, J., "A neural network for the simulation of biological systems", *Journal of Molecular Structure (Theochem)*, Elsevier Science Ltd., Vol. 398-399, Special Issue, 1997, pp. 565-571.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA31						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ31						Yes No
	AK31						Yes No
	AL31						Yes No
	AM31						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

NB	AN	31	Ramos-Nino, M. E. *et al.*, "A comparison of quantitative structure-activity relationships for the effect of benzoic and cinnamic acids on *Listeria monocytogenes* using multiple linear regression, artificial neural network and fuzzy systems", *Journal of Applied Microbiology*, Society for Applied Bacteriology, Vol. 82, No. 2, February 1997, pp. 168-176.
	AO	31	Rogers, D. and Hopfinger, A. J., "Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 34, No. 4, July/August 1994, pp. 854-866.
	AP	31	Sammon, Jr., J. W., "A Nonlinear Mapping for Data Structure Analysis", *IEEE Transactions on Computers*, IEEE, Vol. C-18, No. 5, May 1969, pp. 401-409.
	AQ	31	Simon, Z. *et al.*, "Mapping of Dihydrofolate-reductase Receptor Site by Correlation with Minimal Topological (Steric) Differences", *Journal of Theoretical Biology*, Academic Press, Inc., Vol. 66, No. 3, June 7, 1997, pp. 485-495.
	AR	31	Smellie, A. S. *et al.*, "Fast Drug-Receptor Mapping by Site-Directed Distances: A Novel Method of Predicting New Pharmacological Leads", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 31, No.3, August 1991, pp. 386-392.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA32						
	AB32						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ32						Yes No
	AK32						Yes No
	AL32						Yes No
	AM32						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	32	Specht, D. F., "A General Regression Neural Network", *IEEE Transactions on Neural Networks*, IEEE, Vol. 2, No. 6, November 1991, pp. 568-576.
	AO	32	Svozil, D. *et al.*, "Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter π^H_2", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 2, 1997, pp. 338-342.
	AP	32	Todorov, N. P. and Dean, P. M., "Evaluation of a method for controlling molecular scaffold diversity in de novo ligand design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 11, 1997, pp. 175-192.
	AQ	32	Torgerson, W. S., "Multidimensional Scaling: I. Theory and Method", *Psychometrika*, The Psychometric Society, Vol. 17, No. 4, December 1952, pp. 401-419.
	AR	32	Vapnik, V., "Principles of Risk Minimization for Learning Theory", *Advances in Neural Information Processing Systems 4*, Morgan Kaufmann Publishers, Inc., 1992, pp. 831-838.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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	AA33						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ33						Yes No
	AK33						Yes No
	AL33						Yes No
	AM33						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	33	Vapnik, V. and Bottou, L., "Local Algorithms for Pattern Recognition and Dependencies Estimation", *Neural Computation*, Massachusetts Institute of Technology, Vol. 5, No. 6, November 1993, pp. 893-909.
	AO	33	Viswanadhan, V. N. *et al.*, "Mapping the binding site of the nucleoside transporter protein: a 3D-QSAR study", *Biochimica et Biophysica Acta*, Elsevier Science Publishers B.V., Vol. 1039, No. 3, 1990, pp. 356-366.
	AP	33	Warr, W. A., "Exploiting Molecular Diversity: Small Molecule Libraries for Drug Discovery", Report of Conf rence held in La Jolla, California, Jan. 23-25, 1995.
	AQ	33	Westhead, D. R. *et al.*, "A comparison of heuristic search algorithms for molecular docking", *Journal of Computer-Aided Molecular Design*, Kluwer Academic Publishers, Vol. 11, 1997, pp. 209-228.
	AR	33	Willett, P., "Genetic algorithms in molecular recognition and design", *Trends in Biotechnology*, Elsevier Science Publishers B.V., Vol, 13, No. 12, December 1995, pp. 516-521.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA34						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ34						Yes No
	AK34						Yes No
	AL34						Yes No
	AM34						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	34	Willett, P. and Winterman, V., "A Comparison of Some Measures for the Determination of Inter-Molecular Structural Similarity Measures of Inter-Molecular Structural Similarity", *Quantitative Structure-Activity Relationships*, VCH, Vol. 5, No. 1, March 1986, pp. 18-25.
	AO	34	Zadeh, L. A., "Communication Fuzzy Algorithms", *Information and Control*, Academic Press, Vol. 12, No. 2, February 1968, pp. 94-102.
	AP	34	Zadeh, L. A., "Fuzzy Sets", *Information and Control*, Academic Press, Vol. 8, No. 3, June 1965, pp. 338-353.
	AQ	34	Copy of International Search Report issued April 21, 1998 for Appl. No. PCT/US97/20919, 6 pages.
	AR	34	Copy of International Search Report issued May 13, 1998 for Appl. No. PCT/US97/20918, 7 pages.

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA35						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ35						Yes No
	AK35						Yes No
	AL35						Yes No
	AM35						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	35	Aoyama, T. *et al.*, "Neural Networks Applied to Structure-Activity Relationships," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33., No. 3, 1990, pp. 905-908.
	AO	35	Gasteiger, J. *et al.*, "Analysis of the Reactivity of Single Bonds in Aliphatic Molecules by Statistical and Pattern Recognition Methods," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 33, No. 3, 1993, pp. 385-394.
	AP	35	Guez, A. and Nevo, I., "Neural networks and fuzzy logic in clinical laboratory computing with application to integrated monitoring," Clinica Chimica Acta, Elsevier Science Publishers B.V., Vol. 248, 1996, pp. 73-90.
	AQ	35	Rouvray, D.H., "Similarity in Chemistry: Past, Present and Future," *Topics in Chemistry*, Springer-Verlag, Vol. 173, 1995, pp. 1-30.
	AR	35	de Ridder, D. and Duin, R.P.W., "Sammon's mapping using neural networks: A comparison," *Pattern Recognition Letters*, Elsevier Science Publishers B.V., Vol. 18, No. 11-13, 1997, pp. 1307-1316.

EXAMINER	DATE CONSIDERED
Samuel Brezda	12/03/03

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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	AI36						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ36						Yes No
	AK36						Yes No
	AL36						Yes No
	AM36						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	36	Kim, H. *et al.*, "Self-Organized Distributed Networks for Learning Highly Nonlinear Mapping," *Intelligent Engineering Systems Through Artificial Neural Networks*, American Society of Mechanical Engineers, Vol. 4, November 13-16, 1994, pp. 109-114.
	AO	36	Pal, N.R. and Eluri, V.K., "Two Efficient Connectionist Schemes for Structure Preserving Dimensionality Reduction," *IEEE Transactions on Neural Networks*, IEEE, Vol 9, No. 6, November 1998, pp. 1142-1154.
	AP	36	Domine, D. *et al.*, "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," *Journal of Chemometrics*, John Wiley & Sons, Ltd., Vol. 7, No. 4, July-August 1993, pp. 227-242.
	AQ	36	Hosenpud, J. *et al.*, "The Effect of Transplant Center Volume on Cardiac Transplant: A Report of the United Network for Organ Sharing Scientific Registry," *Journal of the American Medical Association*, American Medical Association, Vol. 271, No. 23, June 15, 1994, pp. 1844-1849.
	AR	36	English-language Abstract of European Patent No. 0 355 628, printed from Dialog File No. 351(February, 1990 - Date of publication of application).

EXAMINER	DATE CONSIDERED
Samuel Broda	12/03/03

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